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Due to a transient quantum interference during a wavepacket collision with a potential barrier, a particular momentum, that depends on the potential parameters but is close to the initial average momentum, becomes suppressed. The hole left pushes the momentum distribution outwards leading to a significant constructive enhancement of lower and higher momenta. This is explained in the momentum complex-plane language in terms of a saddle point and two contiguous “structural” poles, which are not associated with resonances but with incident and transmitted components of the wavefunction.

The traditional formulation of quantum scattering theory in terms of an “ S -matrix” assumes that only the *results* of the collision can be observed at “asymptotic” distances and times, but that the collision itself cannot be observed. This perspective is justified to analyze the products of standard collisions of atomic or molecular beams. But the S -matrix approach is not enough to describe modern experiments where the collision complex can be observed by means of femtosecond laser pulses or “spectroscopy of the transition state” [1]. Also, in quantum kinetic theory of gases accurate treatments must abandon the “completed collision” approximation and use a full description, e.g. in terms of Möller wave operators as in the Waldmann-Snider equation and its generalizations for moderately dense gases [2]. In any case, it is important to understand the collision process itself to control or modify the products. This has motivated a recent trend of theoretical and experimental work to investigate the details of the collision itself, and not only its asymptotics. In particular, a quantum effect has been recently described by Brouard and Muga [3,4] in which the probability to find the particle with a momentum above a given value is larger, in the midst of the collision, than the quantity allowed classically by energy conservation. The effect belongs to a group where the conservation of classical energy seems to be violated. Well known examples are the tunnel effect, or in general the non vanishing probability to find the particle in evanescent regions beyond the classical turning points.

This transient enhancement of the momentum tail may in principle be observed by collisions of ultracold atoms with a laser field that can be turned off suddenly in the time scale of the atomic motion [3], and implies as a macroscopic consequence deviations from the Maxwellian

velocity distribution [5]. We initiated the research of the present work looking for conditions that increase the effect and favor its observability. In so doing we have found an unexpected regime where the effect is much higher than in previously studied cases. In this letter we shall describe such a regime and analyze its physical origin, namely a transient interference between transmission and incidence components of the wavepacket. Let us first review briefly the main aspects of the classically forbidden increase of high-momenta. Brouard and Muga have studied several examples where the quantity

$$G^q(p, t) \equiv \int_p^\infty \{ |\psi(p', t)|^2 - |\psi(p', 0)|^2 \} dp'$$

takes on positive values for positive potentials (the corresponding classical quantity is negative or zero due to energy conservation) [3,4]. An important aspect of this effect is its *transient* character, $G^q \leq 0$ before and after the collision. The effect is also *generic* [3,4], because the stationary components of the wavepacket have, in momentum representation, a tail due to the resolvent which is always present in the Lippmann-Schwinger equation. This tail goes beyond the maximum value allowed by the conservation of energy.

For a Gaussian wavepacket colliding with an infinite wall, maximum values of $G_{max}^q(p, t) \simeq 0.05$ have been reported [3]. Also a “delta” potential was used [4] to analyze the influence of the opacity of the barrier. For the cases examined, an increase of G^q with the opacity was observed up to a saturation level where the infinite wall results were recovered [4]. This suggested that the observability of the effect would improve with strongly opaque conditions. In a complementary study we have systematically varied the spatial variance of the wavepacket, δ_x , and the height of a square barrier, V_0 , for a fixed average initial momentum p_c . We have found, contrary to previous expectations, that the maximum effect corresponds to energies well above the barrier and to large values of δ_x . In this regime the barrier is not at all opaque and essentially the full wave is finally transmitted. Moreover, G_{max}^q is as large as 0.27.

The numerical effort to perform these calculations by ordinary propagation methods (such as the split operator method) is rather heavy, since large values of δ_x and the need to discern fine details of the momentum distribution require an extense and dense grid. In fact for very large values of δ_x this numerical route has to be eventually abandoned. But even if one gets numerical results with

enough computer power, they will not provide any explanation of the unexpectedly high G^a values. Fortunately these two difficulties can be overcome with an approximate analytical solution. Here we shall sketch its obtention, a more detailed account will be given elsewhere. First the momentum representation of the wavefunction is expressed using the basis of stationary eigenstates of H , $|p'^+\rangle$, corresponding to incident momentum p' , and energy $E' = p'^2/(2m)$,

$$\psi(p, t) = \int_{-\infty}^{+\infty} \langle p|p'^+\rangle e^{-iE't/\hbar} \langle p'^+|\psi(t=0)\rangle dp'. \quad (1)$$

If the initial state at time $t = 0$ does not overlap with the potential and has negligible negative momentum components we can write

$$\psi(p, t) = \int_0^{+\infty} \langle p|p'^+\rangle e^{-iE't/\hbar} \langle p'^+|\psi(t=0)\rangle dp'. \quad (2)$$

To facilitate the treatment of the integral in the p' -complex plane we may now extend the lower limit to $-\infty$ using the analytical continuation of $\langle p|p'^+\rangle$, $p' > 0$, over $p' < 0$ (and later over the whole complex plane).

For a square barrier of height V_0 and width d , centered at the coordinate origin, the delta-normalized stationary wavefunction with incident momentum p' is

$$\langle x|p'^+\rangle = \frac{1}{h^{1/2}} \begin{cases} Ie^{ik'x} + Re^{-ik'x}, & x < -d/2 \\ Ce^{ik''x} + De^{-ik''x}, & -d/2 < x < d/2 \\ Te^{ik'x}, & x > d/2, \end{cases} \quad (3)$$

where $I = 1$, $k' = p'/\hbar$ and $k'' = \sqrt{p'^2 - 2mV_0}/\hbar$. The coefficients R, C, D and T are determined by continuity of the wavefunction and its derivative. The momentum representation $\langle p|p'^+\rangle$ will correspondingly have five terms. The terms with I, R and T have poles in the p' -complex momentum plane at

$$\begin{aligned} p'_I &= p + i0 \\ p'_R &= -p - i0 \\ p'_T &= p - i0, \end{aligned} \quad (4)$$

while the terms with C and D do not have these *structural poles* [6], which are not related to resonances or to the potential profile. The four functions R, C, D and T present an infinite series of *resonance and anti-resonance poles* in the third and fourth quadrants due to the zeros of a common denominator

$$\Omega(p') = \cos(k''d) - \frac{i}{2} \left(\frac{k''}{k'} + \frac{k'}{k''} \right) \sin(k''d). \quad (5)$$

(In particular $T(p') = \exp(-ik'd)/\Omega(p')$.) The conditions examined in this work correspond however to “direct scattering”, where these resonance singularities do not play any significant role.

The initial state is taken as a minimum-uncertainty-product Gaussian centered at the position $-\alpha\delta_x$, $\alpha > 0$, with average momentum p_c ,

$$\langle p'|\psi(t=0)\rangle = \left(\frac{2\delta_x}{\pi\hbar^2} \right)^{1/4} e^{-\frac{\delta_x(p'-p_c)^2}{\hbar^2} + \frac{ip'\alpha\delta_x}{\hbar}}. \quad (6)$$

This expression and the momentum representation of (3) are inserted in (2) to obtain five integrals. The full treatment of the resulting integrals follows closely ref. [7]. The integrals with C and D may be evaluated with the steepest descent method for large values of δ_x . The steepest descent path (SDP) is a straight line with slope $-t\hbar/(2m\delta_x)$, with a saddle point close to p_c in the midst of the collision. We shall always assume that the slope is small so that when the integration contour is deformed along this path it “cuts” the resonance poles of the fourth quadrant far from the real axis, and their residues can be neglected (“direct scattering” conditions).

Because of the interference between the saddle and the structural poles, the simple steepest descent treatment valid for C and D is not valid for the other terms. A uniform expression for a smooth treatment of the pole crossing of the SDP is provided by the w -function, $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$, which may also be defined by its integral expression [8]

$$w(z) = \frac{1}{i\pi} \int_{\Gamma_-} du \frac{e^{-u^2}}{u-z}, \quad (7)$$

where Γ_- goes from $-\infty$ to ∞ passing below the pole. Since we are interested in wavepackets with energy well above the barrier maximum the “reflection term” with R may be neglected. The remaining contribution is

$$\psi_{IT} = i\hbar^{-1/2} \hbar\tau \int_{-\infty}^{\infty} [g_I(p') + g_T(p')] e^{\phi(p')} dp', \quad (8)$$

where

$$\begin{aligned} \tau &= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{2\delta_x}{\pi\hbar^2} \right)^{1/4} \\ g_I(p') &= \frac{e^{ipd/2\hbar}}{p - p' + i0} \\ g_T(p') &= \frac{-T(p') \exp[i(2p' - p)d/2\hbar]}{(p - p' - i0)}, \end{aligned}$$

and

$$\phi(p') = \frac{-ip'^2t}{2m\hbar} - \frac{\delta_x(p' - p_c)^2}{\hbar^2} + \frac{ip'(\alpha\delta_x - d/2)}{\hbar}. \quad (9)$$

The functions $g_I(p')$ and $g_T(p')$ present structural poles at p'_I and p'_T ; in addition $g_T(p')$ has resonance and anti-resonance poles.

The SDP is a straight line with the same negative slope as before, passing through the saddle point,

$$s = \frac{m}{4m^2\delta_x^2 + t^2\hbar^2} \{4mp_c\delta_x^2 + (\alpha\delta_x - d/2)\hbar^2t + i2\hbar[m\delta_x(\alpha\delta_x - d/2) - p_c\delta_x t]\}. \quad (10)$$

To integrate (8), the contour is deformed to the SDP passing over the saddle. The same reasons to neglect the residues from the resonance poles in the C and D terms are now applicable. To introduce the w -functions, the integrand must be put in the form (7). We complete the square in (9) and use the change of variable

$$u = \frac{p' - s}{f}, \quad f = \left(\frac{\delta_x}{\hbar^2} + i \frac{t}{2m\hbar} \right)^{-1/2} \quad (11)$$

to obtain

$$\langle p|\psi(t)\rangle \simeq i f \tau \hbar^{-1/2} \hbar e^{-(\delta_x p_c^2/\hbar^2) + \eta^2} \times \int_{-\infty}^{\infty} [g_I(u) + g_T(u)] e^{-u^2} du,$$

where $g(u) \equiv g(p'(u))$, and

$$\eta = \left(\frac{2p_c\delta_x}{\hbar^2} + i \frac{(\alpha\delta_x - d/2)}{\hbar} \right) \left[4 \left(\frac{\delta_x}{\hbar^2} + i \frac{t}{2m\hbar} \right) \right]^{-1/2}.$$

We may retain the main contribution from g_I from its behaviour near the pole by approximating $g_I(u) \approx \mathcal{R}_I/(u - u_I)$, where \mathcal{R}_I is residue of $g_I(u)$ at the point $u = u_I = (p'_I - l)/f$, and similarly for g_T . For an approximate expression of $\langle p|\psi\rangle$, and considering that the wave is much more extended in space than the barrier we may neglect the contribution from C and D and retain only the incidence and transmission terms,

$$\langle p|\psi(t)\rangle \simeq \hbar^{-1/2} \pi \tau \hbar e^{-(\delta_x p_c^2/\hbar^2) + \eta^2} e^{ipd/2\hbar} \times [w(u_I) + T(p)w(-u_T)] \equiv \psi_{IT}^0(p, t). \quad (12)$$

A more precise expression including a term ψ_{RCD} and corrections to the zeroth order ψ_{IT}^0 is given elsewhere and allows to obtain the wave function and G_{max}^q accurately for large values of δ_x with small computational effort. However (12) captures the essential, and provides a simple, explanatory picture of the phenomenon we want to discuss.

Fig. 1 shows the distribution of momenta $|\langle p|\psi(t)\rangle|^2$ for different instants of time, from the initial one to a time after the collision has been completed, passing through the instant where $G^q = 0.27$ is maximum. In all figures the numerical values correspond to collisions of ultracold Rubidium atoms with an effective laser potential. The observed behaviour does not have a classical explanation. Note that the wavepacket is considerably broader than the barrier. A classical ensemble of particles with the same Gaussian phase-space (Wigner) distribution as (6) would only be slightly deformed due to the small fraction of particles located on the barrier at a given time, and would keep the maximum at the average momentum

p_c . Moreover, there could not be any spectacular acceleration or deceleration as the one seen in the two peaks of the quantum momentum distribution. We shall see that the zero of the quantum momentum distribution, which forbids in this case the initially dominant momentum p_c , is due to a destructive interference whereas the two new peaks correspond to momentum regions of constructive interference.

In Fig. 2 the *Argand diagrams* of the two terms are represented, namely the imaginary versus the real parts obtained by varying p at equal intervals. Each lobule corresponds to one of the terms. The “motion” as p increases begins close to the origin, downwards in both diagrams. The left peak of the momentum distribution corresponds to the zone where the two moduli increase together and are approximately in phase. After the descending motion there is a fast, approximately circular motion where the phases become opposed (destructive interference). Finally, the two curves meet again *in phase* in the upper part of the lobules, this momentum interval corresponds to the right peak of the momentum distribution. The described behaviour is essentially due to the two w -functions $w(u_I)$ y $-w(-u_T)$, as shown in Fig. 3, where the two Argand diagrams of the two w -functions and of the factors that multiply them are represented between the momenta of the two maxima. Clearly the effect of the factors, whose phases remain essentially constant around π , is simply to invert the two lobules of the ws . The fast motion of the w -functions is due to the pass of the two contiguous structural poles $u_I = (p + i0)/f$ and $u_T = (p - i0)/f$ near the saddle point at $u = 0$. A sweep from smaller to larger values of p moves the couple of poles along the real p' axis from left to right, while, for fixed t , the saddle point and the steepest descent path do not depend of p . Since $u_I \approx u_T$ we can write, using the relation between w -functions of argument of opposite sign, see (7),

$$w(u_I) = e^{-u_I^2} - w(-u_T). \quad (13)$$

During the collision, the saddle point is very close to the real axis of the p' -plane, only slightly below in Fig. 4, and the slope of the SDP is very small. This means that the difference between the two w -contributions is essentially a *real* exponential, which implies a “simultaneous motion”, with equal imaginary parts, along the two lobules of the Argand diagram. The rapid variation of the phases of the ws when passing close to the saddle point follows from its integral expression (7). When u_I passes close to $u = 0$ and close to the real axis of the u -plane, the denominator is essentially real and changes its sign quickly, so there is a rapid change by π in the phases of $w(u_I)$ and $-w(-u_T)$. The phase opposition alone does not explain however why the interference is totally destructive. It is also necessary to have equal moduli of the two incidence and transmission terms of (12) for an exact cancellation. Actually the equality is obtained only

transitorily, since before and after the collision only one lobule remains, the one for incidence before the collision, and the one for transmission after the collision. Along the collision the incident lobule decreases and the transmission one grows, until they equilibrate and give a perfect cancellation and the two constructive interference zones of Fig. 1.

By changing the barrier height the fases of the factors that multiply the ws change, the lobules rotate with respect to each other, and one of the two in-phase regions grows while the other diminishes, so that the two peaks of the momentum distribution become asymmetric, see Figures 5 and 6, where the momentum distributions and the corresponding lobules of the Argand diagrams are shown, compare also with Fig. 2. Note that these factors do not depend on time and therefore the angle between the lobules remains constant throughout the collision. This means that the positions of the maxima and minima do not change significantly for a given collision.

An important point is that the interference effect described does not depend critically on the square barrier potential, and we have observed it in particular for a Gaussian barrier. Note that the arguments leading to Eq. (12) are in fact of general validity and independent of the potential shape, with $-d/2$ and $d/2$ being points where the potential may be assumed to be essentially zero, and T being the corresponding transmission amplitude. The possibility to observe this effect with ultracold atoms rests on the ability to prepare appropriate initial states. Turning off the laser potential during the collision will leave a two peaked momentum distribution that implies at later times a visible spatial separation between two wave components, one faster than the other.

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FIG. 1. $|\langle p|\psi(t)\rangle|^2$ for different values of t : $t = 0$ (dotted-dashed line); $t = 2.333 t_u$ (solid line); $t = 2.731 t_u$ (dashed line); and $t = 3.233 t_u$ (dotted line). $m = 1.558023 m_u$, $V_0 = 102.5 e_u$, $d = 2.5 l_u$, $-\alpha\delta_x = -50 l_u$, $\delta_x = 107.99 l_u^2$, with an average momentum $p_c = 28.48 p_u$ well above the classical threshold $(2mV_0)^{1/2} = 17.87 p_u$. The units are scaled for numerical convenience in the computations as $e_u = 10^{-13}$ a.u. of energy, $p_u = 10^{-4}$ a.u. of momentum, $l_u = 2 \times 10^6$ a.u. of length, $m_u = 10^5$ a.u. of mass, and $t_u = 2 \times 10^{15}$ a.u. of time.

FIG. 2. Imaginary versus real parts of the incident contribution to $\psi_{IT}^0(p, t)$ (empty circles), and of the transmission contribution (filled circles), for $t = 2.731 t_u$ and different values of p equally spaced between $p = 28 p_u$ and $p = 29 p_u$. Other parameters as in Fig. 1.

FIG. 3. Imaginary versus real parts of $\omega(u_I)$ (empty circles) and $-\omega(-u_T)$ (filled circles) for $t = 2.731 t_u$ and different values of p equally spaced between the two peaks of Fig. 1, see the text. The prefactors corresponding to $\omega(u_I)$ and $-\omega(-u_T)$ in $\psi_{IT}^0(p, t)$ are also shown for the same momentum interval, solid and dashed lines respectively. Other parameters as in Fig. 1.

FIG. 4. Integration contour in the complex p' -plane when the SDP crosses the pair of structural poles p'_I and p'_T . Also shown the structural pole p'_R , the saddle point of equation (10), and the incident average momentum p_c .

FIG. 5. $|\langle p|\psi(t)\rangle|^2$ as a function of p , for two different values of V_0 : $102.5 e_u$ (solid line), and $105 e_u$ (dashed line). The value of t is selected to get the maximum effect, $G^q \simeq 0.24$; $t = 2.731 t_u$. Other parameters as in Fig. 1.

FIG. 6. Imaginary versus real parts of the incident contribution to $\psi_{IT}^0(p, t)$ (empty circles), and of the transmission contribution (filled circles), for $V_0 = 105 e_u$, the value of t for which the effect is maximum ($t = 2.731 t_u$), and different values of p . Other parameters as in Fig. 1.

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Figure captions









